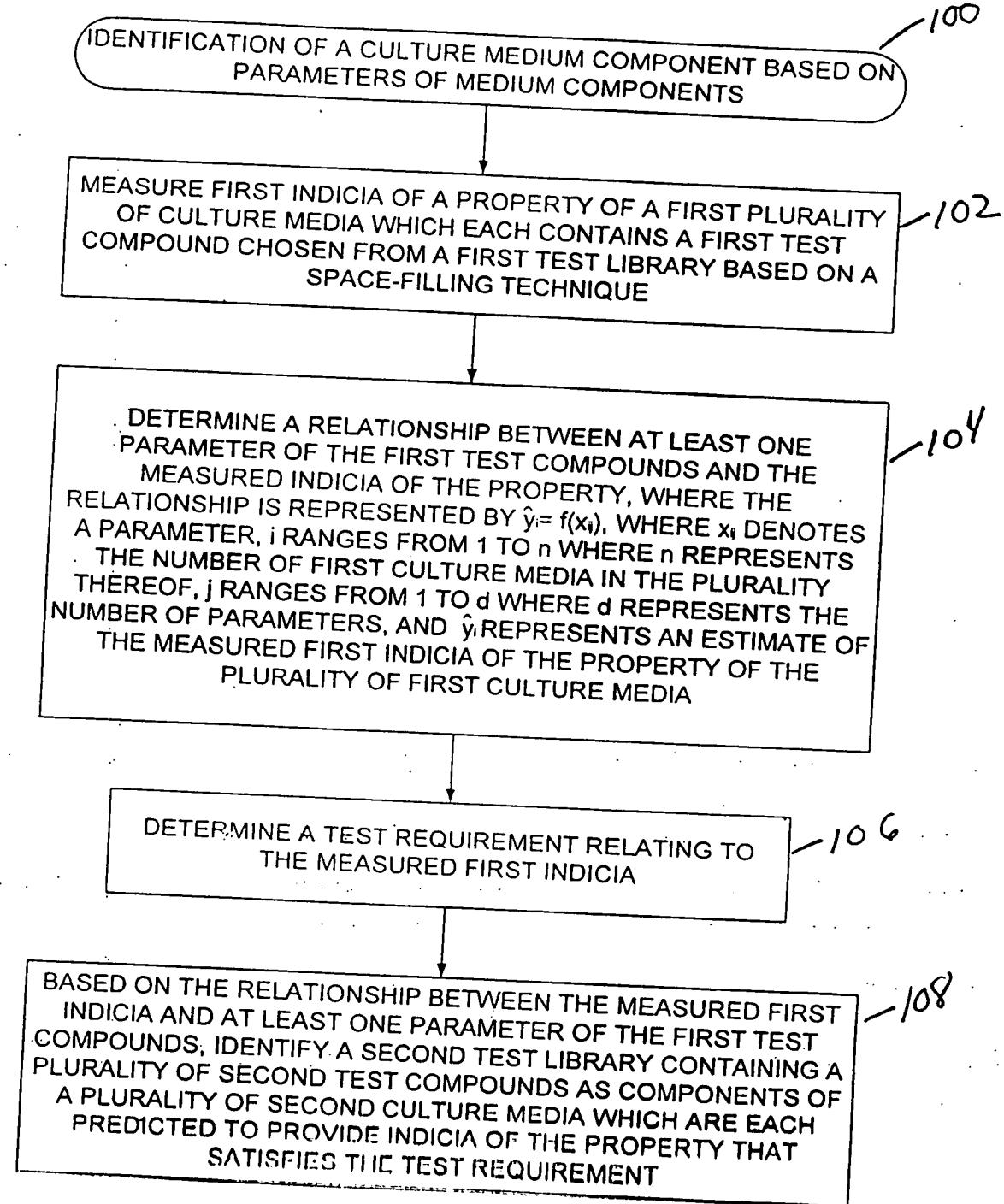


PRINT OF DRAWIN  
AS ORIGINALLY F...D



**FIG. 1**

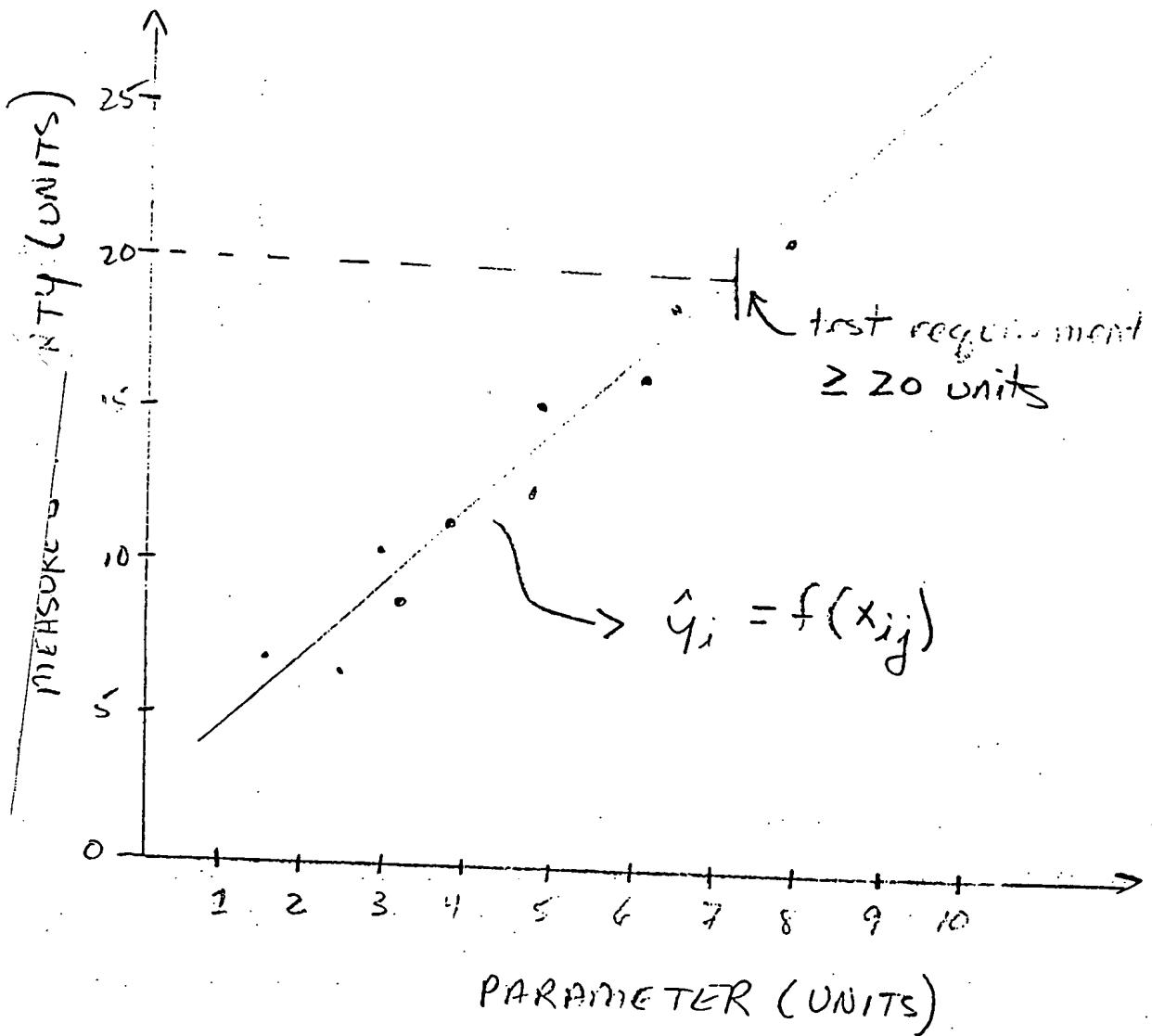


FIG. 2

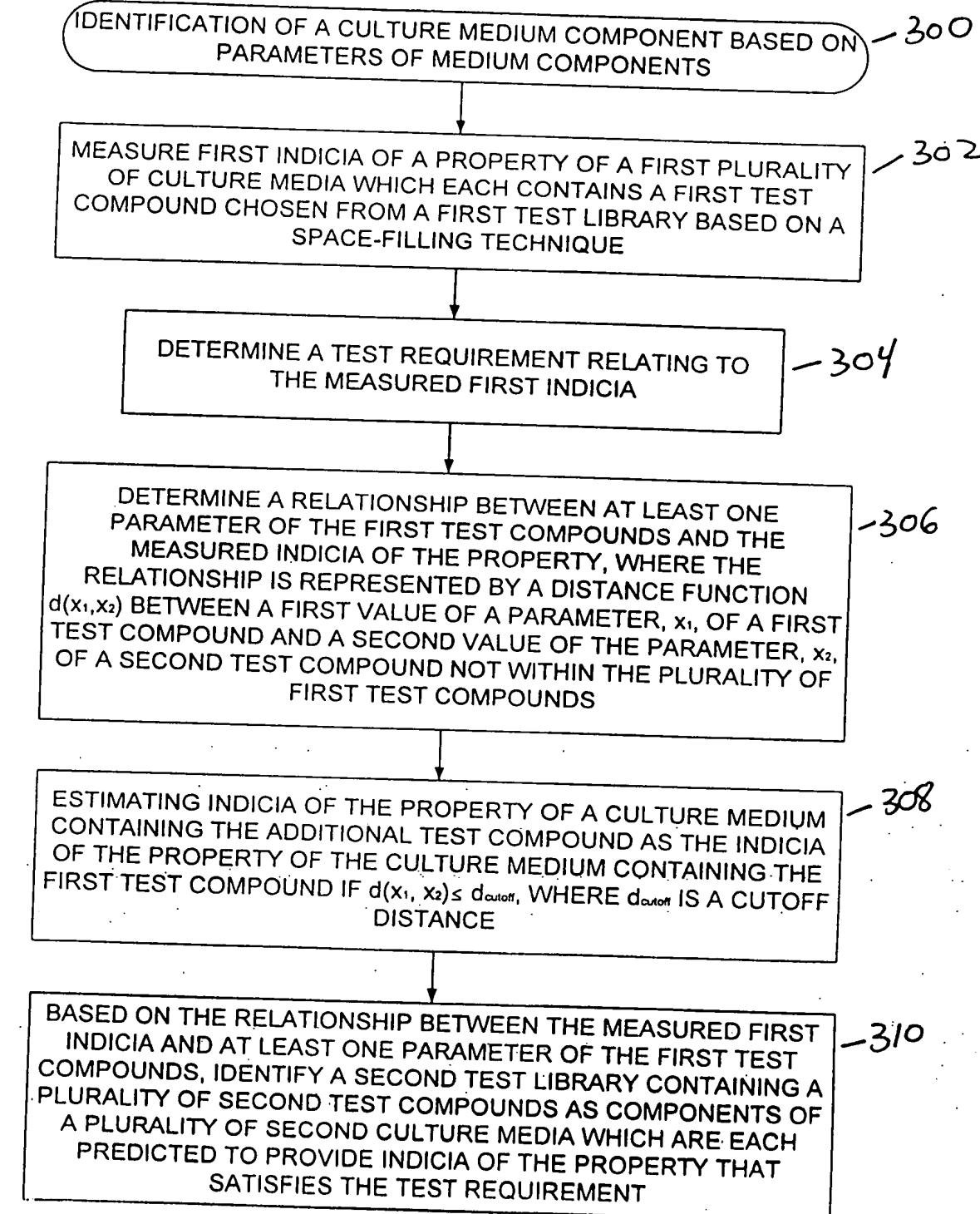


FIG. 3

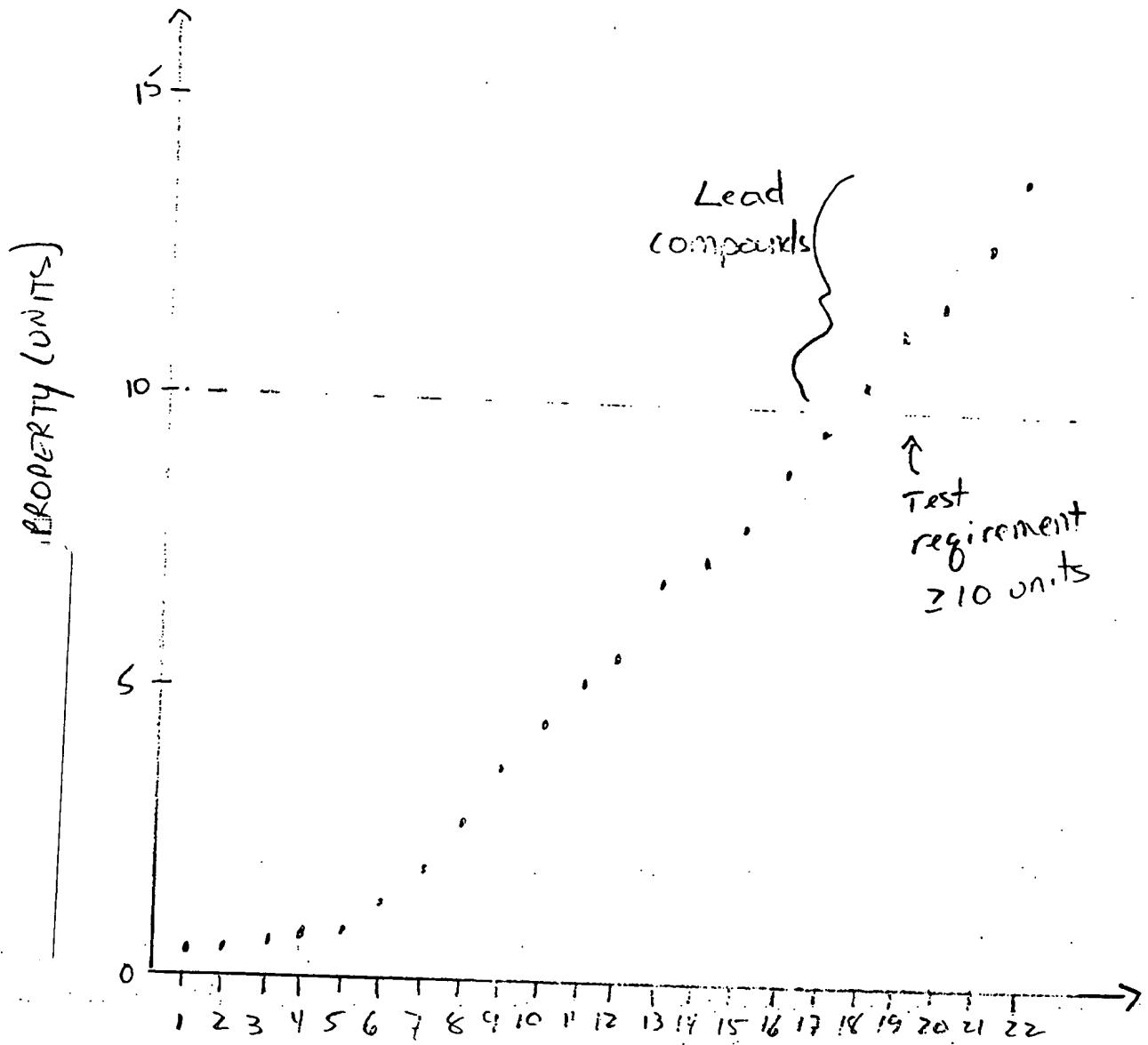


FIG 4A

PRINT OF DRAWING  
AS ORIGINATED

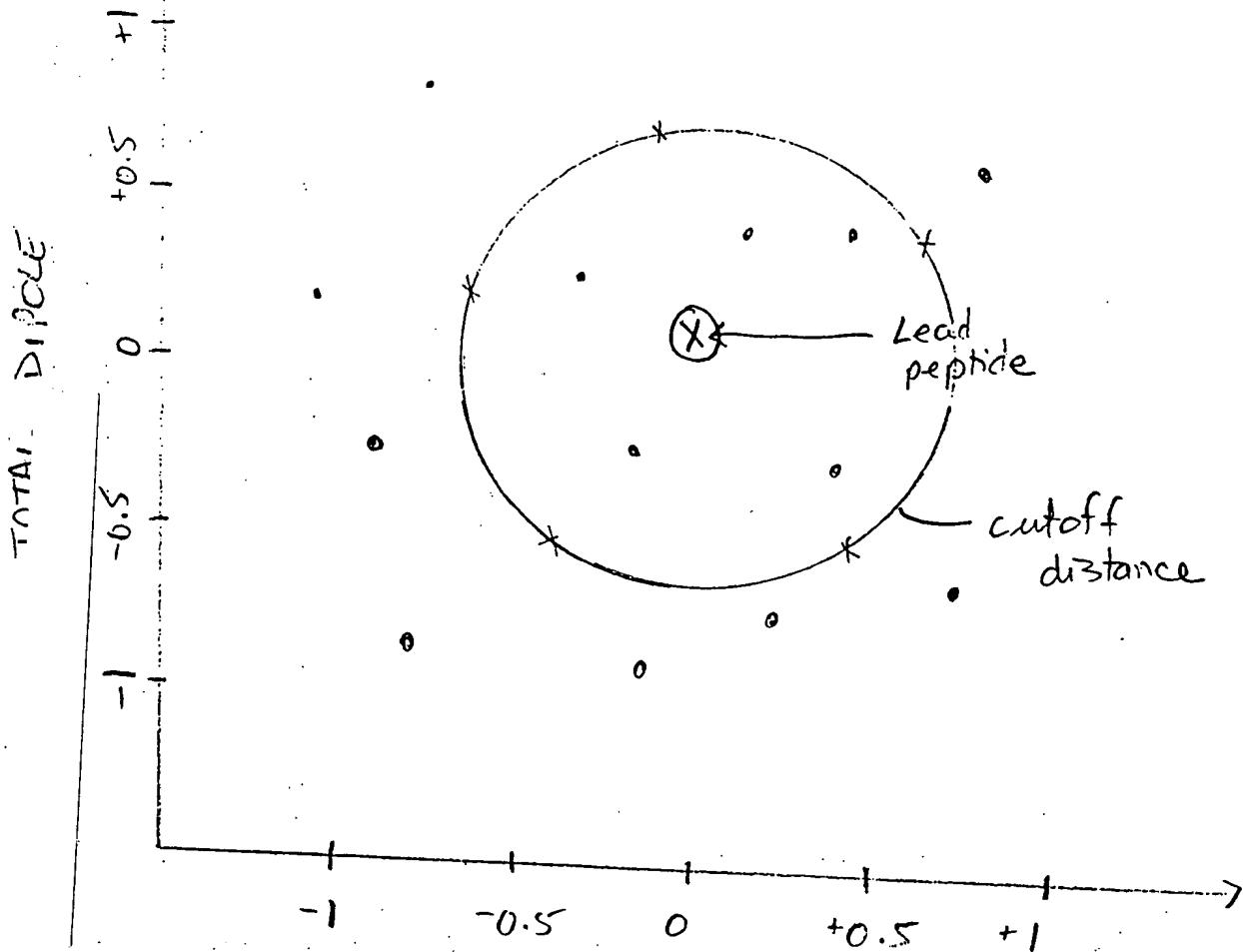


FIG. 4B

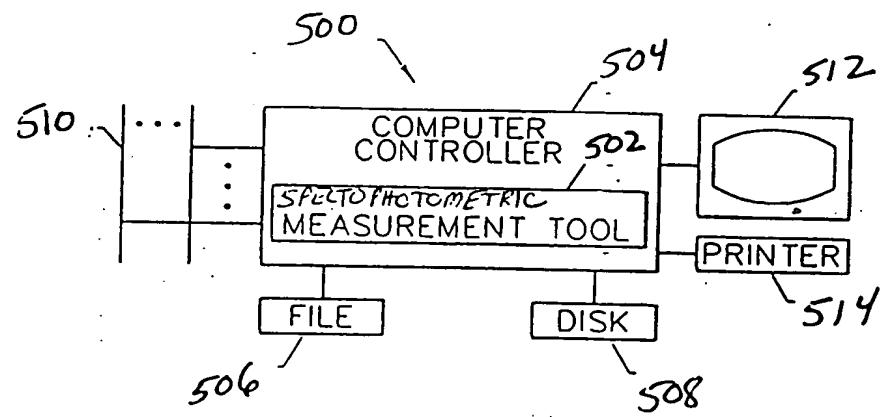


FIG. 5

60

FORMATION OF A REPRESENTATIVE COMPOUND LIBRARY BASED ON WHOLE MOLECULE PARAMETERS

60<sup>2</sup>

REPRESENT EACH OF A PLURALITY OF GROUPS OF COMPOUND ISOMERS FROM WITHIN A COMPOUND SPACE AS A RESPECTIVE CANDIDATE COMPOUND BASED ON AT LEAST ONE SHARED GLOBAL PARAMETER

60<sup>4</sup>

EXPAND LESS THAN ALL OF THE CANDIDATE COMPOUNDS INTO THEIR CONSTITUENT COMPOUND ISOMERS USING A SPACE-FILLING DESIGN

60<sup>6</sup>

DEFINE A TEST LIBRARY CONTAINING LESS THAN ALL OF THE EXPANDED COMPOUND ISOMERS

FIG. 6

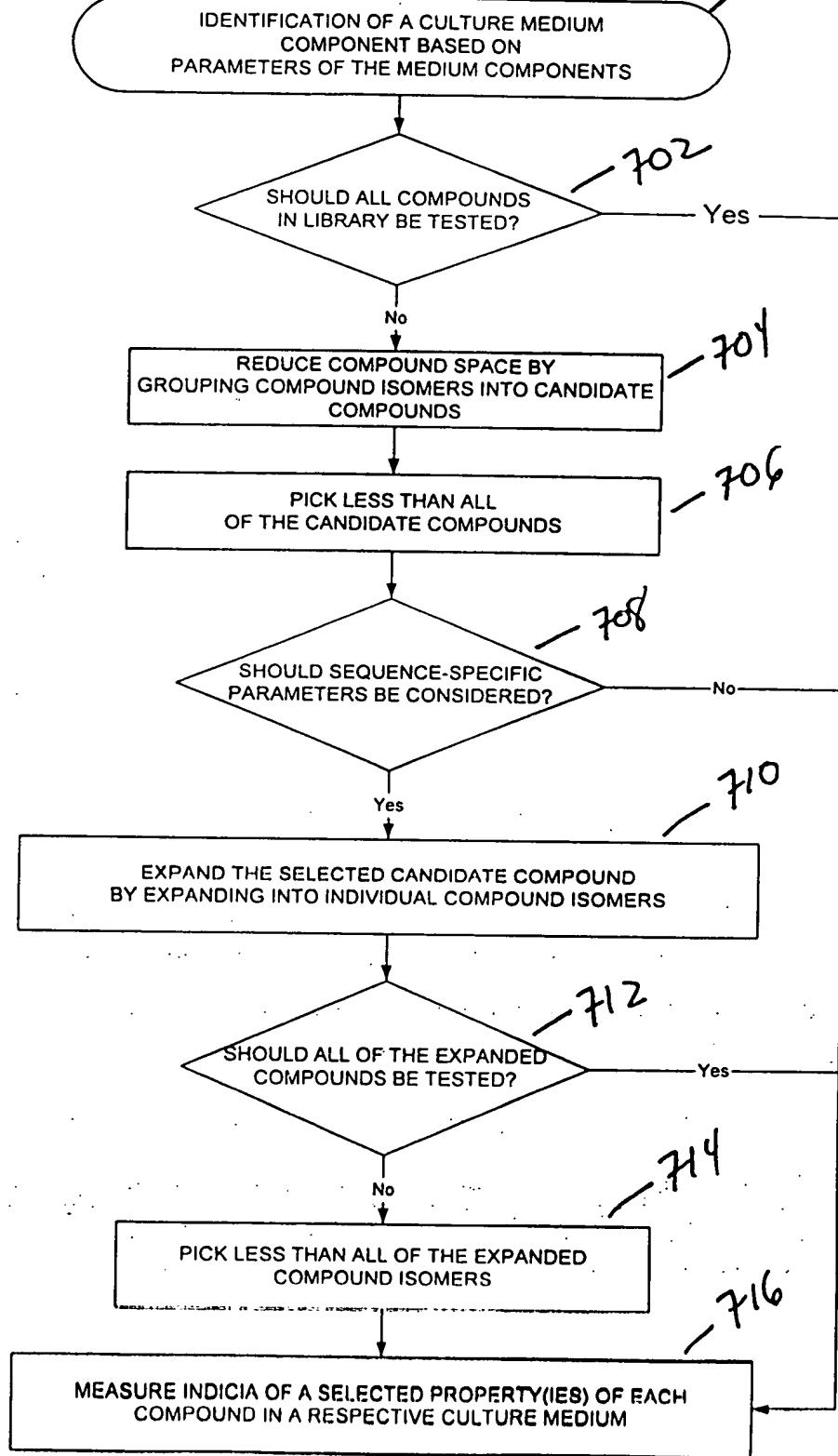


FIG. 7

PREDICTION OF THE BIOLOGICAL ACTIVITY OF A PEPTIDE BASED ON  
WHOLE MOLECULE PARAMETERS OF THE PEPTIDE

MEASURING INDICIA OF A BIOLOGICAL ACTIVITY OF A PLURALITY OF TEST  
PEPTIDES CHOSEN FROM A FIRST TEST PEPTIDE LIBRARY BASED ON A  
SPACE-FILLING DESIGN

DETERMINING A RELATIONSHIP BETWEEN THE MEASURED INDICIA OF THE  
BIOLOGICAL ACTIVITY AND AT LEAST ONE WHOLE MOLECULE PARAMETER OF  
THE PLURALITY OF TEST PEPTIDES

PREDICTING THE INDICIA OF THE BIOLOGICAL ACTIVITY OF A PEPTIDE NOT  
WITHIN THE PLURALITY OF TEST PEPTIDES BASED ON THE RELATIONSHIP

FIG. 8